Symbolic integration with respect to the Haar measure on the unitary group in *Mathematica*

Zbigniew Puchała, Jarosław Adam Miszczak

Institute of Theoretical and Applied Informatics, Polish Academy of Sciences, Bałtycka 5, 44-100 Gliwice, Poland

Abstract

We present `IntU` package for *Mathematica* computer algebra system. The presented package performs a symbolic integration of polynomial functions over the unitary group with respect to unique normalized Haar measure. We describe a number of special cases which can be used to optimize the calculation speed for some classes of integrals. We also provide some examples of usage of the presented package.

Keywords: unitary group, CUE, symbolic integration

PROGRAM SUMMARY

Manuscript Title: Symbolic integration with respect to the Haar measure on THE unitary group in *Mathematica*
Authors: Z. Puchała, J.A. Miszczak
Program Title: `IntU`
Journal Reference:
Catalogue identifier:
Licensing provisions: GPLv3
Programming language: Mathematica 8
Computer: Any computer supporting Mathematica 8
Operating system: Any operating system capable of running Mathematica 8 or higher, *e.g.* GNU/Linux, MacOS X, Microsoft Windows XP or higher
RAM: For examples listed in the paper the program uses less than 20 MB (less than 45 MB with *Mathematica* front-end)

Email addresses: `z.puchala@iitis.pl` (Zbigniew Puchała), `miszczak@iitis.pl` (Jarosław Adam Miszczak)

Keywords: unitary group, CUE, symbolic integration
PACS: 03.67.-a, 02.70.Wz, 02.10.Ox .
Classification: 5
Nature of problem: Symbolic integration of polynomial functions over the unitary group with respect to unique normalized Haar measure.
Solution method: A package of functions for *Mathematica* computer algebra system.
Restrictions: Running time of the presented procedures grows rapidly with the dimensionality of the problem.
Running time: For examples listed in the paper the running time is shorter than 20 sec.

1. Introduction

The integration over unitary group is an important subject of studies in many areas of science, including mathematical physics, random matrix theory and algebraic combinatorics. In 2006 Collins and Śniady [1] proved a formula for calculating monomial integrals with respect to the Haar measure on the Unitary group

$$\int_{\mathrm{U}(d)} U_{IJ}\overline{U}_{I'J'}dU = \int_{\mathrm{U}(d)} U_{i_1j_1}\dots U_{i_nj_n}\overline{U}_{i'_1j'_1}\dots\overline{U}_{i'_nj'_n}dU. \tag{1}$$

Integrals of the above type are known as *moments of the* $\mathrm{U}(d)$ and are well-known in mathematical physics literature for a long time. The problem of the integration of elements of unitary matrices was for the first time considered in the context of nuclear physics in [2]. The asymptotic behaviour of the integrals of the type (1) was considered by Weingarten in [3].

In this paper we describe a *Mathematica* package `IntU` [4] for calculating polynomial integrals over $\mathrm{U}(d)$ with respect to the Haar measure. We describe a number of special cases which can be used to optimize the calculation speed for some classes of integrals. We also provide some examples of usage of the presented package including the applications in the study of the geometry of the quantum states.

This paper is organised as follows. In Section 2 we introduce notation present mathematical background concerning polynomial integrals over unitary group. In Section 3 we describe some special cases, in which the in-

tegration can be calculated more efficiently. In Section 4 we provide the description of the `IntU` package with the list of main functions. In Section 5 we show some examples of the usage. In Section 6 we provide a summary of the presented results and give conclusions.

2. Mathematical background

2.1. Basic concepts

We denote by $\mathcal{M}_n$ square matrices of size n. The compact group of $d \times d$ unitary matrices we denote as $\mathrm{U}(d)$. We equip the above group with unique normalized Haar measure denoted by dU. Random elements distributed with measure dU form so called *Circular Unitary Ensemble*.

Integer partition λ of a positive integer n is a weakly decreasing sequence $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_l)$ of positive integers, such that $\sum_{i=1}^{l} \lambda_i = |\lambda| = n$. To denote that λ is a partition of n we write $\lambda \vdash n$. The length of a partition is denoted by $l(\lambda)$. By $\lambda \sqcup \mu$ we denote a partition of $n_1 + n_2$ obtained by joining partitions $\lambda \vdash n_1$ and $\mu \vdash n_2$.

Each permutation $\sigma \in S_n$ can be uniquely decomposed into a sum of disjoint cycles where the lengths of the cycles sum up to n. Thus the vector of the lengths of the cycles, after reordering, forms a partition $\lambda \vdash n$. The partition λ is called the cycle type of permutation σ.

2.2. Moments of the $\mathrm{U}(d)$

Let us consider a polynomial p. From the linearity of an integral we have

$$\int_{\mathrm{U}(d)} p(U) dU = \sum_{I,J,I',J'} c(I,J,I',J') \int_{\mathrm{U}(d)} U_{IJ} \overline{U}_{I'J'} dU, \tag{2}$$

where I, J, I', J' are multi-indices and c are the coefficients of p. The value of such monomial integrals is given as [1]

$$\begin{aligned} \int_{\mathrm{U}(d)} U_{IJ} \overline{U}_{I'J'} dU &= \int_{\mathrm{U}(d)} U_{i_1 j_1} \ldots U_{i_n j_n} \overline{U}_{i'_1 j'_1} \ldots \overline{U}_{i'_n j'_n} dU = \\ &= \sum_{\sigma,\tau \in S_n} \delta_{i_1, i'_{\sigma(1)}} \ldots \delta_{i_n, i'_{\sigma(n)}} \delta_{j_1, j'_{\tau(1)}} \ldots \delta_{j_n, j'_{\tau(n)}} \mathcal{W}g(\tau\sigma^{-1}, d), \end{aligned} \tag{3}$$

where $\mathcal{W}g$ is the Weingarten function discussed below. In the case where the multi-indices differ in length, *i.e.* $n \neq n'$, we have

$$\int_{\mathrm{U}(d)} U_{IJ}\overline{U}_{I'J'}dU = \int_{\mathrm{U}(d)} U_{i_1j_1}\dots U_{i_nj_n}\overline{U}_{i'_1j'_1}\dots\overline{U}_{i'_{n'}j'_{n'}}dU = 0. \quad (4)$$

The integrals of the above type are known as *moments of the* $\mathrm{U}(d)$.

2.3. Weingarten function

The *Weingarten function* [1] is defined for $\sigma \in S_n$ and positive integer d, as

$$\mathcal{W}g(\sigma, d) = \frac{1}{(n!)^2} \sum_{\substack{\lambda \vdash n \\ l(\lambda) \leq d}} \frac{\chi^\lambda(e)^2}{s_{\lambda,d}(1)} \chi^\lambda(\sigma), \quad (5)$$

where the sum is taken over all integer partitions of n with length $l(\lambda) \leq d$, $s_{\lambda,d}(1)$ is the Schur polynomial s_λ evaluated at $(\underbrace{1, 1, \dots, 1}_{d})$ and χ^λ is an irreducible character of the symmetric group S_n indexed by partition λ.

2.3.1. The dimension of irreducible representation of $\mathrm{U}(d)$

The value of the Schur polynomial at the point $(\underbrace{1, 1, \dots, 1}_{d})$, *i.e.* the dimension of irreducible representation of $\mathrm{U}(d)$ corresponding to partition λ, is equal to (see *e.g.* [5, Theorem 6.3])

$$s_{\lambda,d}(1) = s_\lambda(\underbrace{1, 1, \dots, 1}_{d}) = \prod_{1 \leq i < j \leq d} \frac{\lambda_i - \lambda_j + j - i}{j - i}. \quad (6)$$

2.3.2. Irreducible character of S_n

The irreducible character of S_n indexed by partition λ, $\chi^\lambda(\sigma)$ depends on a conjugacy class of permutation σ. Two permutations are in the same conjugacy class if and only if they have the same cycle type, thus it is common to write $\chi^\lambda(\sigma) = \chi^\lambda(\mu)$, where μ is an integer partition corresponding to the cycle type of σ.

In the case of identity permutation the cycle type is given by a trivial partition, $e = \{\underbrace{1, 1, \dots, 1}_{n}\}$, and the character value is equal to the dimension of the irreducible representation of S_n indexed by λ. In this case it is given

by the celebrated *hook length* formula [5, Eq. 4.12]

$$\chi^{\lambda}(e) = \frac{|\lambda|!}{\prod_{i,j} h^{\lambda}_{i,j}}, \tag{7}$$

where $|\lambda| = \lambda_1 + \lambda_2 + \cdots + \lambda_{l(\lambda)}$, and $h^{\lambda}_{i,j}$ is the hook length of the cell (i, j) in a Ferrers diagram corresponding to partition λ, see *e.g.* [6, p. 57].

In the case of a non-trivial partition the character of symmetric group $\chi^{\lambda}(\sigma) = \chi^{\lambda}(\mu)$ can be evaluated with the use of Murnaghan-Nakayama rule (see *e.g.* [7, Th. 4.10.2]), which describes a combinatorial way of calculating the character. [8] is used.

From the above considerations one can notice that the Weingarten function depends only on a cycle type of a permutation σ and thus it is constant on a conjugacy class represented by σ. Thus we may define the Weingarten function as

$$\mathcal{W}g(\mu, d) = \frac{1}{(|\mu|!)^2} \sum_{\substack{\lambda \vdash |\mu| \\ l(\lambda) \leq d}} \frac{\chi^{\lambda}(e)^2}{s_{\lambda,d}(1)} \chi^{\lambda}(\mu), \tag{8}$$

where μ is an integer partition, which is a cycle type of σ.

3. Special cases

In this section we present some special cases of integrals, with respect to the Haar measure on the unitary group. In these cases the value of the integral can be calculated without the direct usage of formula (3), which requires processing of $\prod_i^d k_i! \prod_j^d l_j!$ permutations, where k_i (l_j) denotes the number of i (j) in multi-indices I (J) respectively.

The presented special cases have been implemented in the package, to increase its efficiency. This goal has been achieved by minimizing the number of calculations of the Weingarten function.

3.1. First two moments of $\mathrm{U}(d)$

In the case of monomials of rank equal to 2 and 4, we have the following formulas [9, Prop. 4.2.3]

$$
\begin{aligned}
\int_{\mathrm{U}(d)} u_{ij}\overline{u}_{i'j'} dU &= \frac{1}{d}\delta_{ii'}\delta_{jj'}, && (9)\\
\int_{\mathrm{U}(d)} u_{i_1j_1}u_{i_2j_2}\overline{u}_{i'_1j'_1}\overline{u}_{i'_2j'_2} dU &= \frac{\delta_{i_1i'_1}\delta_{i_2i'_2}\delta_{j_1j'_1}\delta_{j_2j'_2} + \delta_{i_1i'_2}\delta_{i_2i'_1}\delta_{j_1j'_2}\delta_{j_2j'_1}}{d^2-1} && (10)\\
&- \frac{\delta_{i_1i'_1}\delta_{i_2i'_2}\delta_{j_1j'_2}\delta_{j_2j'_1} + \delta_{i_1i'_2}\delta_{i_2i'_1}\delta_{j_1j'_1}\delta_{j_2j'_2}}{d\,(d^2-1)},
\end{aligned}
$$

allowing us to calculate the values of polynomial integrals of degree less than 5 without the direct usage of the formula (3).

This optimization gives only a minor improvement of efficiency, as in these cases the direct calculation of Weingarten function is very fast.

3.2. Elements from one row (column)

The next optimization is based on the fact that the distribution of random vector consisting of squares of absolute values of a row (or a column) of unitary matrix distributed with the Haar measure, is uniform on a standard d-simplex Δ^d [9, Ch. 4]

$$\{|u_{i,1}|^2, |u_{i,2}|^2, \dots, |u_{i,d}|^2\} \sim \mathbb{U}(\Delta^d), \tag{11}$$

where $\mathbb{U}(A)$ denotes the normalized uniform measure (proportional to Lebesgue measure) on a set $A \subset \mathbb{R}^d$, and standard d-simplex Δ^d is defined as, $\Delta^d = \{\lambda \in \mathbb{R}^d : \lambda_i \geq 0, \sum_{i=1}^d \lambda_i = 1\}$.

Using Beta integral, one obtains that for a fixed row i_0 and a vector p with non-negative entries p_j, we have the following

$$\int_{\mathrm{U}(d)} \prod_{j=1}^{d} |u_{i_0,j}|^{2p_j} dU = \Gamma(d)\frac{\Gamma(p_1+1)\times\cdots\times\Gamma(p_d+1)}{\Gamma(p_1+\cdots+p_d+d)}. \tag{12}$$

The above, as a special case, gives us:

$$\begin{aligned}\int_{\mathrm{U}(d)} |u_{i_0,j}|^{2k} dU &= \frac{(d-1)!k!}{(d-1+k)!}, &(13)\\ \int_{\mathrm{U}(d)} |u_{i_0,j}|^2 |u_{i_0,k}|^2 dU &= \frac{1}{d(d+1)}, &(14)\end{aligned}$$

which can be found in literature [9, 10].

This optimization allows for an enormous improvement in efficiency thanks to avoiding $(\sum p_i)! \prod p_i!$ executions of Weingarten function needed in the case of the direct usage of formula (3).

3.3. Even powers of diagonal element absolute values

In this subsection we consider the integrals of the type

$$\int_{\mathrm{U}(d)} |u_{i,j}|^{2p} |u_{k,l}|^{2q} dU, \tag{15}$$

where p, q are non-negative integers and $i \neq k$, $j \neq l$. In the case of $p = q = 1$ this integral is known [9, Prop. 4.2.3]

$$\int_{\mathrm{U}(d)} |u_{i,j}|^2 |u_{k,l}|^2 dU = \frac{1}{d^2-1}. \tag{16}$$

For general non-negative integers p, q the following proposition is true.

Proposition 1. *Let p, q be non-negative integers, for $i \neq k$ and $j \neq l$, we have*

$$\int_{\mathrm{U}(d)} |u_{i,j}|^{2p} |u_{k,l}|^{2q} dU = p!q! \sum_{\substack{\lambda \vdash p \\ \mu \vdash q}} \mathbf{k}_\lambda \mathbf{k}_\mu \mathcal{W}g(\lambda \sqcup \mu, d), \tag{17}$$

where the above sum is taken over all integer partitions of p and q. Symbol $\mathbf{k}_\nu$ denotes a cardinality of conjugacy class for a permutation with cycle type given by partition $\nu \vdash r$ [7, Eq. 1.2]

$$\mathbf{k}_\nu = \frac{r!}{1^{m_1} m_1! 2^{m_2} m_2! \cdots r^{m_r} m_r!}, \tag{18}$$

where m_i denotes the number of i in partition ν.

The above is a special case of more general fact.

Proposition 2. *For any permutation $\pi \in S_d$ and any non-negative integers $p_1, p_2, \dots p_d$, we have*

$$
\begin{aligned}
\int_{\mathrm{U}(d)} \prod_{j=1}^{d} |u_{j,\pi(j)}|^{2p_j} dU &= \int_{\mathrm{U}(d)} \prod_{j=1}^{d} |u_{j,j}|^{2p_j} dU \qquad (19)\\
&= \left(\prod_{j=1}^{d} p_j!\right) \sum_{\lambda_1 \vdash p_1} \sum_{\lambda_2 \vdash p_2} \cdots \sum_{\lambda_d \vdash p_d} \left(\prod_{j=1}^{d} \mathbf{k}_{\lambda_j}\right) \mathcal{W}g(\lambda_1 \sqcup \lambda_2 \sqcup \cdots \sqcup \lambda_d, d).
\end{aligned}
$$

Proof. If we apply the formula from Eq. (3) to integral (19), then the non-vanishing permutations of indices are these which permute within the blocks of sizes $\{p_1, p_2, \dots, p_d\}$, *i.e.*

$$\sigma = \sigma_1 \oplus \sigma_2 \oplus \cdots \oplus \sigma_d,$$

where $\sigma_j \in S_{p_j}$ and it permutes indices in j^{th} block of size p_j. The same situation holds in the case of the second indices. Thus the permutation $\tau\sigma^{-1}$ is also in this form. Each permutation of the above type will be present in the sum $\prod_{j=1}^{d} p_j!$ times. The cycle type of such permutations is given by a partition which is obtained by joining cycle types of small permutations. Since Weingarten function depends only on a cycle type of permutation, the size of conjugacy class is calculated for each partition, instead of evaluating multiple times Weingarten function. □

The formula (19) is far less computationally demanding than the direct usage of (3). One can notice that Proposition 2 allows us to avoid at least $\prod_{j=1}^{d} p_j!$ executions of Weingarten function comparing to the direct usage of (3). However, the exact time-efficiency depends also on the cardinality of conjugacy classes for partitions of $p_1, \dots, p_d$.

3.4. Cycle permutations

In this section we consider another special type of integral for positive integer k and a permutation σ of $\{1, 2, \dots, m\}$ being a cycle

$$\int_{\mathrm{U}(d)} \left(\prod_{i=1}^{m} u_{i,i}\overline{u}_{i,\sigma(i)}\right)^k dU. \qquad (20)$$

We have the following proposition.

Proposition 3. *Let $m \leq d$, k is a positive integer and $\sigma \in S_m$ be a cycle,* i.e. *the cycle type is given by partition $\{m\}$. Then*

$$\int_{\mathrm{U}(d)} \left(\prod_{i=1}^{m} u_{i,i} \overline{u}_{i,\sigma(i)} \right)^k dU = (k!)^{2m-1} \sum_{\lambda \vdash k} \mathbf{k}_\lambda \mathcal{W}g(m\lambda, d). \tag{21}$$

Proof. One can notice that cycle lengths of permutations in this setting must be divisible by m. The number of permutations with cycle type given by a particular partition can be easily obtained by the usual counting argument. □

Using the above formula (21) one obtains an enormous improvement in efficiency by avoiding more than $(k!)^{2m-1}$ executions of Weingarten function, comparing to the case of the direct usage of (3).

4. Package description

Below we describe the functions implemented in `IntU` package. The functions are grouped in three categories: functions implementing the main functionality, functions related to the calculation of Weingarten function and helper functions.

4.1. Main functionality

The main functionalty of `IntU` package is provided be the `IntegrateUnitaryHaar` and `IntegrateUnitaryHaarIndices` functions. The first one operates directly on polynomial expressions, while the second one accepts four-tuple of indices. The examples of the usage are given in Section 5.

- `IntegrateUnitaryHaar[integrand,{var,dim}]` – gives the definite integral on unitary group with respect to the Haar measure, accepting the following arguments
  - `integrand` – the polynomial type expression of variable `var` with indices placed as subscripts, can contain any other symbolic expression of other variables,
  - `var` – the symbol of variable for integration,
  - `dim` – the dimension of a unitary group, must be a positive integer.

  This function is presented in the examples described in Sections 5.1, 5.3 and 5.5.

- `IntegrateUnitaryHaar[f,{u,d1},{v,d2},...]` – gives multiple integral
$$\int_{\mathrm{U}(\mathtt{d1})} dU \int_{\mathrm{U}(\mathtt{d2})} dV \ldots \mathtt{f}. \tag{22}$$
This function is presented in the example described in Section 5.4.

- `IntegrateUnitaryHaarIndices[{I1,J1,I2,J2},dim]` – calculates the integral in Eq. (3) for given multi-indices `I1,J1,I2,J2` and the dimension `dim` of the unitary group. This function is presented in the example described in Section 5.2.

4.2. Weingarten function

The main functions implemented in the package, `IntegrateUnitaryHaar` and `IntegrateUnitaryHaarIndices`, utilize the following functions to find the value of the integral.

- `Weingarten[type,dim]` – returns the value of the Weingarten function given in Eq. (8) and accepts the following arguments
  - `type` – an integer partition which corresponds to cycle type of permutation (see Section 2.3),
  - `dim` – the dimension of a unitary group, must be a positive integer.

- `CharacterSymmetricGroup[part,type]` – gives the character of the symmetric group $\chi^{\mathtt{part}}(\mathtt{type})$ (see Section 2.3.2).

  Parameter `type` is optional. The default value is set to a trivial partition and in this case the function returns the dimension of the irreducible representation of symmetric group indexed by `part`, given by Eq. (7). If `type` is specified the value of the character is calculated by Murnaghan-Nakayama rule using `MNInner` algorithm provided in [8].

- `SchurPolynomialAt1[part,dim]` – returns the value of the Schur polynomial $s_{\mathtt{part}}$ at point $(\underbrace{1, 1, \ldots, 1}_{\mathtt{dim}})$, *i.e.* the dimension of irreducible representation of $\mathrm{U}(\mathtt{dim})$ corresponding to `part`, see Eq. (6).

4.3. Helper functions

- `PermutationTypePartition[perm]` – gives the partition which represents the cycle type of the permutation `perm` (see Section 2.1).

- `MultinomialBeta[p]` - for a given d-dimensional vector of non-negative numbers $p_1, p_2, \ldots, p_d$ returns the value of multinomial Beta function defined as
$$B(p) = \frac{\prod_{i=1}^{d} \Gamma(p_i)}{\Gamma(\sum_{i=1}^{d} p_i)}. \tag{23}$$
This function is used in the optimization described in Section 3.2.

- `ConjugatePartition[part]` – gives a conjugate of a partition `part` (see [5]). This function is used for calculating hook-length formula given by Eq. (7).

- `CardinalityConjugacyClassPartition[part]` – gives a cardinality of a conjugacy class for the permutation with cycle type given by partition `part` (see [7, Eq. 1.2]). This function is used in the optimization described in Section 3.3.

- `BinaryPartition[part]` – gives a binary representation of a partition `part`. This function is needed for the implementation of `MNInner` algorithm.

5. Usage examples

In order to present the main features of the described package we provide a series of examples.

5.1. Elementary integrals

Let us assume that $d = 3$. We want to calculate the following integrals
$$\int_{\mathrm{U}(d)} |u_{1,1}|^2 dU, \tag{24}$$
$$\int_{\mathrm{U}(d)} |u_{1,1}|^2 |u_{2,2}|^2 dU, \tag{25}$$
$$\int_{\mathrm{U}(d)} u_{1,1} u_{2,2} \overline{u}_{1,2} \overline{u}_{2,1} dU. \tag{26}$$

Let us start by initializing the package

```
In[1]:= << IntU`
        Package IntU version 0.2.0 (last modification: 19/09/2011).
```

ow we calculate the integrals.

```
In[2]:= d = 3;

In[3]:= IntegrateUnitaryHaar[Abs[u_{1,1}]^2, {u, d}]

Out[3]= 1/3

In[4]:= IntegrateUnitaryHaar[Abs[u_{1,1} u_{2,2}]^2 , {u, d}]

Out[4]= 1/8

In[5]:= IntegrateUnitaryHaar[u_{1,1} u_{2,2} Conjugate[u_{1,2} u_{2,1}], {u, d}]

Out[5]= -1/24
```

5.2. Operations on indices

Let us take the following set of multi-indices

$$I = \{1, 1, 1, 2, 2\}, \qquad J = \{2, 2, 1, 1, 1\} \tag{27}$$

$$I' = \{1, 1, 1, 2, 2\}, \qquad J' = \{2, 1, 1, 2, 1\} \tag{28}$$

and set $d = 6$. The above is equivalent to expression

$$u_{1,2}u_{1,2}u_{1,1}u_{2,1}u_{2,1}\overline{u}_{1,2}\overline{u}_{1,1}\overline{u}_{1,1}\overline{u}_{2,2}\overline{u}_{2,1} \tag{29}$$

with symbolic variable u, which we aim to integrate over $\mathrm{U}(d)$. After simplification the expression is equal to

$$|u_{1,1}|^2|u_{1,2}|^2|u_{2,1}|^2u_{1,2}u_{2,1}\overline{u}_{1,1}\overline{u}_{2,2}. \tag{30}$$

After initializing the package and defining appropriate indices

```
In[2]:= I1 = {1, 1, 1, 2, 2}; J1 = {2, 2, 1, 1, 1};
        I2 = {1, 1, 1, 2, 2}; J2 = {2, 1, 1, 2, 1};
        d = 6;
```

we calculate the integral using `IntegrateUnitaryHaarIndices` as

```
In[5]:= IntegrateUnitaryHaarIndices[{I1, J1, I2, J2}, d]
```

$$\text{Out[5]=}\ -\frac{1}{16\,200}$$

which is equivalent to

```
In[6]:= IntegrateUnitaryHaar[
          Abs[u_{1,1} u_{1,2} u_{2,1}]^2 u_{1,2} u_{2,1} Conjugate[u_{1,1} u_{2,2}], {u, d}]
```

$$\text{Out[6]=}\ -\frac{1}{16\,200}$$

5.3. Matrix expressions

IntU package allows us to integrate matrix expressions, for example let us take $d = 2$ and integrate

$$\int_{\mathrm{U}(d)} U^{\otimes 2} \otimes \bar{U}^{\otimes 2} dU. \tag{31}$$

We define symbolic matrices $U \in \mathrm{U}(d)$ and $U2 = U \otimes U \in \mathrm{U}(d^2)$ as

```
In[2]:= d = 2;
        U = Array[u_{#1,#2} &, {d, d}];
        U2 = KroneckerProduct[U, U];
```

and construct the integrand as

```
In[5]:= integrand = KroneckerProduct[U2, Conjugate[U2]];
```

By using IntegrateUnitaryHaar function

```
In[6]:= IntegrateUnitaryHaar[integrand, {u, d}]
```

we learn that the integral in Eq. (31) is equal to

$$\begin{pmatrix}
\frac{1}{3} & 0 & 0 & 0 & 0 & \frac{1}{6} & \frac{1}{6} & 0 & 0 & \frac{1}{6} & \frac{1}{6} & 0 & 0 & 0 & 0 & \frac{1}{3} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{6} & 0 & 0 & 0 & 0 & \frac{1}{3} & -\frac{1}{6} & 0 & 0 & -\frac{1}{6} & \frac{1}{3} & 0 & 0 & 0 & 0 & \frac{1}{6} \\
\frac{1}{6} & 0 & 0 & 0 & 0 & -\frac{1}{6} & \frac{1}{3} & 0 & 0 & \frac{1}{3} & -\frac{1}{6} & 0 & 0 & 0 & 0 & \frac{1}{6} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{6} & 0 & 0 & 0 & 0 & -\frac{1}{6} & \frac{1}{3} & 0 & 0 & \frac{1}{3} & -\frac{1}{6} & 0 & 0 & 0 & 0 & \frac{1}{6} \\
\frac{1}{6} & 0 & 0 & 0 & 0 & \frac{1}{3} & -\frac{1}{6} & 0 & 0 & -\frac{1}{6} & \frac{1}{3} & 0 & 0 & 0 & 0 & \frac{1}{6} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{3} & 0 & 0 & 0 & 0 & \frac{1}{6} & \frac{1}{6} & 0 & 0 & \frac{1}{6} & \frac{1}{6} & 0 & 0 & 0 & 0 & \frac{1}{3}
\end{pmatrix}. \tag{32}$$

5.4. Mean value of local unitary orbit

In this example we calculate the mean value of a local unitary orbit of a given matrix $X \in \mathcal{M}_{d^2}$

$$\mathbb{E}[(U \otimes V)X(U \otimes V)^\dagger]. \tag{33}$$

We assume that U and V are stochastically independent random unitary matrices of size d distributed with the Haar measure. In this case we have

$$\mathbb{E}[(U \otimes V)X(U \otimes V)^\dagger] = \int_{\mathrm{U}(d)} \int_{\mathrm{U}(d)} (U \otimes V)X(U \otimes V)^\dagger dU dV. \tag{34}$$

In this example we take $d = 3$.

We define symbolic matrices X of size d^2 and $U, V \in \mathrm{U}(d)$ as

```
In[2]:= d = 3;
        X = Array[x#1,#2 &, {d^2, d^2}];
        U = Array[u#1,#2 &, {d, d}];
        V = Array[v#1,#2 &, {d, d}];
```

Using `IntegrateUnitaryHaar` function with two variable specifications we calculate the double integral

```
In[6]:= int = IntegrateUnitaryHaar[
          KroneckerProduct[U, V].X.KroneckerProduct[U, V]†
          , {u, d}, {v, d}]
```

and find out that the expectation value in Eq. (33) is equal to

$$\mathbb{E}[(U \otimes V)X(U \otimes V)^\dagger] = \frac{1}{d^2} \mathrm{tr} X \; \mathbb{1}_{d \times d}. \tag{35}$$

Similarly one can calculate the covariance tensor of the local unitary orbit of a given matrix $X \in \mathcal{M}_{d^2}$. If $z = (U \otimes V)X(U \otimes V)^\dagger$ then the covariance tensor is given by [11]

$$\mathbb{E}[\{z_{ij}\overline{z}_{kl}\}_{ijkl}] = \mathbb{E}[(U \otimes V)X(U \otimes V)^\dagger \otimes \overline{(U \otimes V)X(U \otimes V)^\dagger}]. \tag{36}$$

Using `IntegrateUnitaryHaar` one can check that for the fixed dimension the integral agrees with the calculations presented in [11].

5.5. Moments of maximally entangled numerical shadow

If U is a random $d \times d$ unitary matrix distributed according to the Haar measure then the pure state obtained by vectorization $|\xi\rangle = \frac{1}{\sqrt{d}}\mathrm{vec}(U)$ is

maximally entangled on $\mathcal{H}_A \otimes \mathcal{H}_B = \mathbb{C}^d \otimes \mathbb{C}^d$. Moreover, state $|\xi\rangle$ has a distribution invariant to multiplication by local unitary matrices. We denote the corresponding probability measure on pure states of size $d \times d$ as μ. The numerical shadow of operator $X \in \mathcal{M}_{d^2}$ with respect to this measure (maximally entangled numerical shadow) is defined as

$$P_X(z) = \int_{\mathbb{C}^{d^2}} \delta(z - \langle\psi|X|\psi\rangle)\ \mathrm{d}\mu(\psi). \tag{37}$$

The corresponding probability measure is denoted by $d\mu_X^{\mathcal{E}}$. For definition and basic facts concerning numerical shadows see [11, 12, 13].

The first two moments of $d\mu_X^{\mathcal{E}}$ are calculated in [11], and are given by

$$\int_{\mathbb{C}} z\ d\mu_X^{\mathcal{E}}(z) = \frac{1}{d^2}\mathrm{tr}X\ , \tag{38}$$

and

$$\begin{aligned}\int_{\mathbb{C}} z\overline{z}\ d\mu_X^{\mathcal{E}}(z) &= \frac{1}{d^2(d^2-1)}\left(|\mathrm{tr}X|^2 + \|X\|_{\mathrm{HS}}^2\right) \\ &- \frac{1}{d^3(d^2-1)}\left(\|\mathrm{tr}_A(X)\|_{\mathrm{HS}}^2 + \|\mathrm{tr}_B(X)\|_{\mathrm{HS}}^2\right),\end{aligned} \tag{39}$$

where tr_A and tr_B denote partial traces over a specified sub-system and $\|\cdot\|_{\mathrm{HS}}$ is a Hilbert-Schmidt norm given by $\|X\|_{\mathrm{HS}} = \sqrt{\mathrm{tr}XX^\dagger}$.

In order to calculate (39) and (39) define symbolic matrices

```
In[2]:= d = 3;
        X = Array[x#1,#2 &, {d^2, d^2}];
        U = Array[u#1,#2 &, {d, d}];
        ξ = 1/Sqrt[d] Flatten[U];
        z = ξ.X.Conjugate[ξ];
        zz = Simplify[z Conjugate[z]];
```

Now we calculate the first moment

```
In[8]:= IntegrateUnitaryHaar[z, {u, d}]
```

and the second moment

```
In[9]:= IntegrateUnitaryHaar[zz, {u, d}]
```

After some algebraic manipulations one can see that the above agrees with Eqs. (38) and (39).

6. Summary

We described `IntU` package for *Mathematica* computing system for calculating polynomial integrals over $\mathrm{U}(d)$ with respect to Haar measure. We described some number of special cases which can be used to optimize the calculation speed for some classes of integrals. We also provide some examples of the usage of the presented package including the applications in the geometry of the quantum states.

Calculation time of the package strongly depends on a degree of the integrand. For polynomials of small degree the package is able to calculate the value of integral using the direct formula (3). For polynomials of large degree the calculation time grows rapidly and the calculation is possible only if one of the special cases (optimizations) is used.

Nevertheless, the presented package can be very useful in the investigations involving Circular Unitary Ensemble and the geometry of quantum states.

7. Acknowledgements

Work of Z. Puchała was partially supported by the Polish National Science Centre under the research project N N514 513340 while work of J. A. Miszczak was partially supported by the Polish National Science Centre under the research project N N516 475440. Authors would like to thank K. Życzkowski and P. Gawron for motivation and interesting discussions.

References

[1] B. Collins, P. Śniady, Integration with respect to the haar measure on unitary, orthogonal and symplectic group, Commun. Math. Phys. 264 (2006) 773–795. `arXiv:math-ph/0402073`, `doi:10.1007/s00220-006-1554-3`.

[2] N. Ullah, C. Porter, Expectation value fluctuations in the unitary ensemble, Physical Review 132 (2) (1963) 948.

[3] D. Weingarten, Asymptotic behavior of group integrals in the limit of infinite rank, Journal of Mathematical Physics 19 (1978) 999.

[4] Z. Puchała, J. A. Miszczak, IntU package for Mathematica, Software freely available at `http://zksi.iitis.pl/wiki/projects:intu` (2011).

[5] W. Fulton, J. Harris, Representation theory: a first course, Vol. 129 of Graduate Texts in Mathematics, Springer Verlag, 1991.

[6] G. James, A. Kerber, The representation theory of the symmetric group, encyclopaedia of mathematics, vol .16 (1981).

[7] B. Sagan, The symmetric group: representations, combinatorial algorithms, and symmetric functions, Vol. 203, Springer Verlag, 2001.

[8] D. Bernstein, The computational complexity of rules for the character table of S_n, Journal of Symbolic Computation 37 (6) (2004) 727–748.

[9] F. Hiai, D. Petz, The semicircle law, free random variables and entropy, no. 77, Amer Mathematical Society, 2006.

[10] C. Donati-Martin, A. Rouault, Truncations of haar unitary matrices, traces and bivariate brownian bridge, Arxiv preprint arXiv:1007.1366.

[11] Z. Puchała, J. A. Miszczak, P. Gawron, C. F. Dunkl, J. A. Holbrook, K. Życzkowski, Restricted numerical shadow and geometry of quantum entanglement, in preparation (2011).

[12] C. F. Dunkl, P. Gawron, J. A. Holbrook, Z. Puchała, K. Życzkowski, Numerical shadows: measures and densities on the numerical range, Linear Algebra Appl. 434 (2011) 2042–2080. `doi:10.1016/j.laa.2010.12.003`.

[13] C. F. Dunkl, P. Gawron, J. A. Holbrook, J. A. Miszczak, Z. Puchała, K. Życzkowski, Numerical shadow and geometry of quantum states, J. Phys. A: Math. Theor. 44 (33) (2011) 335301. `doi:10.1088/1751-8113/44/33/335301`.